This dataset contains data produced at the University of Leeds:

Analytical characterisation of the complexes (CHN microanalysis).

Electrospray mass spectra (plotted spectra).

X-ray Crystallographic data:

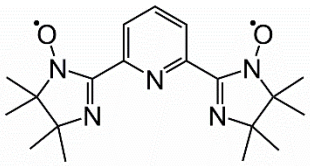
- Structure of $L^3 \cdot 5H_2O$ (CCDC 1911909).
- Structure of **2**·*n*$MeNO_2$ (CCDC 1911991).

Magnetic susceptibility data (raw and plotted data).

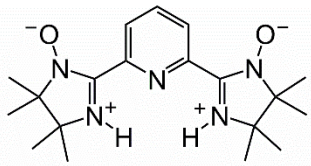
Density functional energy minimisation calculations (SPARTAN format).

The density functional exchange constant calculations in the published study associated with this dataset belong to Dr S. Sproules (University of Glasgow).

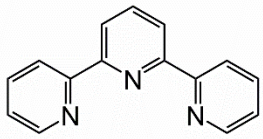
Ligands referred to in this dataset



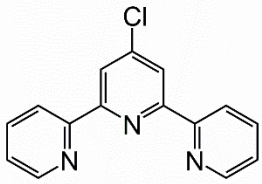
2,6-bis{1-oxyl-4,4,5,5-tetramethyl-4,5-dihydro-1*H*-imidazol-2-yl}pyridine
L^1



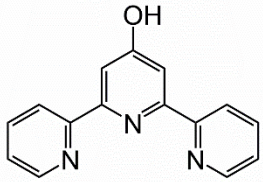
2,6-bis(4,5-dihydro-1-hydroxy-4,4,5,5-tetramethyl-1*H*-imidazol-2-yl)pyridine
L^3



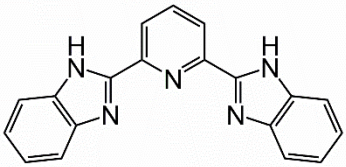
2,2':6',2''-terpyridine
terpy



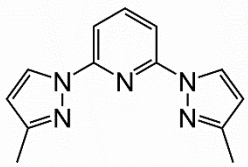
4-chloro-2,2':6',2''-terpyridine
terpyCl



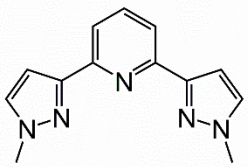
4-hydroxy-2,2':6',2''-terpyridine
terpyOH



2,6-*bis*(1*H*-benzimidazol-2-yl)pyridine
bzimpy

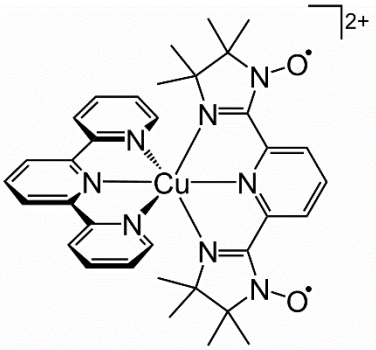


2,6-*bis*(3-methylpyrazol-1-yl)pyridine
Me_2-1-bpp

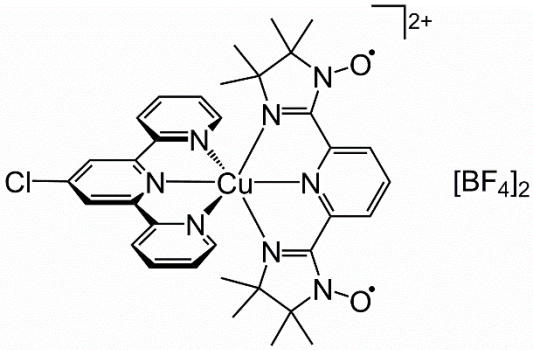


2,6-*bis*(1-methylpyrazol-3-yl)pyridine
Me_2-3-bpp

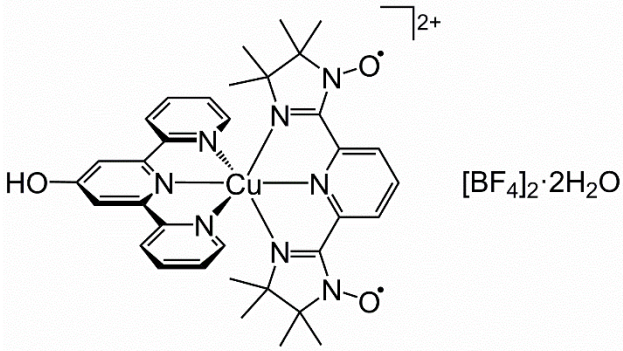
Complexes prepared during this study



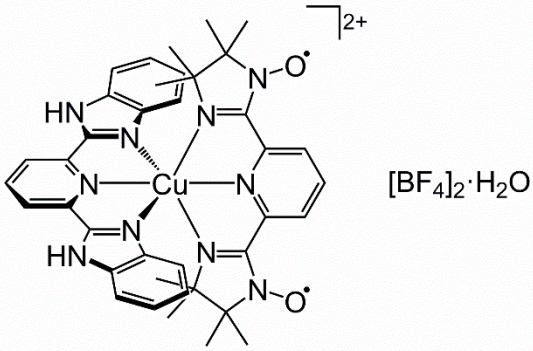
1
$[Cu(terpy)L^1][BF_4]_2$
$C_{34}H_{38}B_2CuF_8N_8O_2$



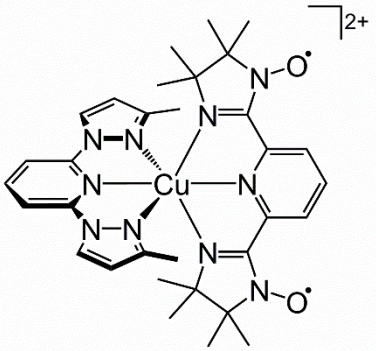
2
$[Cu(terpyCl)L^1][BF_4]_2$
$C_{34}H_{37}B_2ClCuF_8N_8O_2$



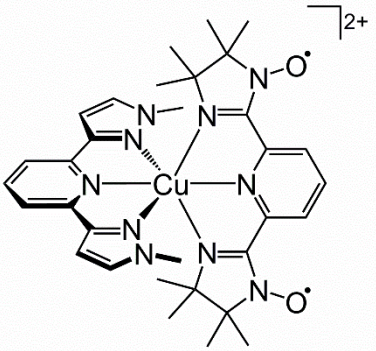
3·$2H_2O$
$[Cu(terpyOH)L^1][BF_4]_2 \cdot 2H_2O$
$C_{34}H_{38}B_2CuF_8N_8O_3 \cdot 2H_2O$



4·H_2O
$[Cu(bzimpy)L^1][BF_4]_2 \cdot H_2O$
$C_{38}H_{40}B_2CuF_8N_{10}O_2 \cdot H_2O$

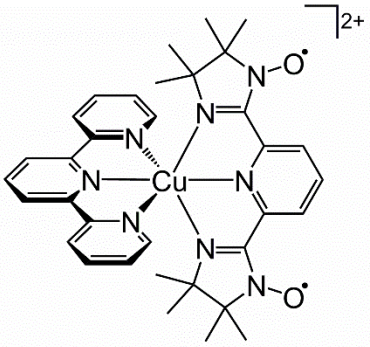


5
$[Cu(Me_2\text{-}1\text{-}bpp)L^1][BF_4]_2$
$C_{32}H_{40}B_2CuF_8N_{10}O_2$



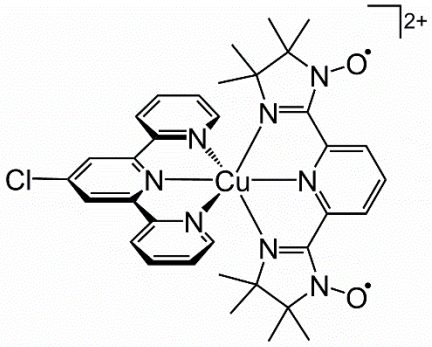
6·$2H_2O$
$[Cu(Me_2\text{-}3\text{-}bpp)L^1][BF_4]_2 \cdot 2H_2O$
$C_{32}H_{40}B_2CuF_8N_{10}O_2 \cdot 2H_2O$

Molecules calculated in the computational study



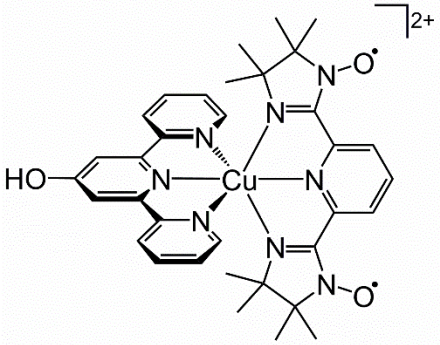
1^{2+}

$C_{34}H_{38}CuN_8O_2$



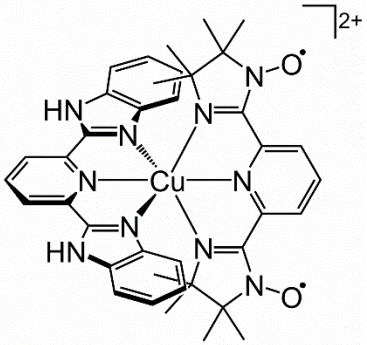
2^{2+}

$C_{34}H_{37}ClCuN_8O_2$



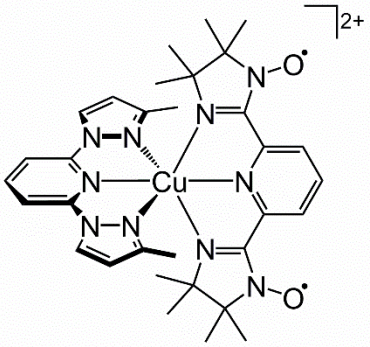
3^{2+}

$C_{34}H_{38}CuN_8O_3$



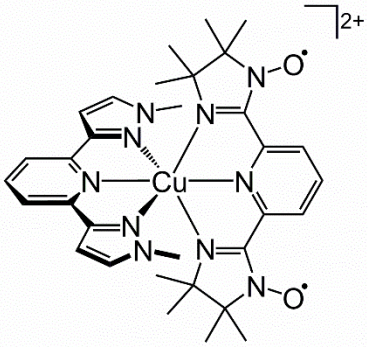
4^{2+}

$C_{38}H_{40}CuN_{10}O_2$



5^{2+}

$C_{32}H_{40}CuN_{10}O_2$



6^{2+}

$C_{32}H_{40}CuN_{10}O_2$